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8-(Pyrimidin-2-ylsulfanylmethyl)quinoline

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The title nitrogen-containing heterocyclic thioether compound, $C_{14}H_{11}N_3S$, adopts a *gauche* conformation; the quinolyl and pyrimidinyl groups are oriented essentially orthogonally.

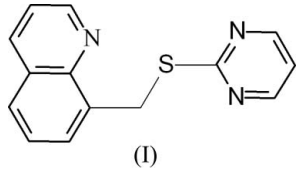
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.095
Data-to-parameter ratio = 13.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Second-order nonlinear optical materials can be obtained through rational design of coordination architectures. Evans & Lin (2002) developed the crystal-engineering strategies to synthesize non-centrosymmetric coordination networks with desired topologies by taking advantage of well defined metal coordination geometries combined with carefully designed asymmetric ligands. We are also attempting to obtain a series of asymmetric quinolyl thioether derivatives as bridging units for construction of coordination polymers. Recently we prepared the title compound, (I). We present here the crystal structure of (I).



(I)

The molecule of (I) adopts a *gauche* conformation. The quinolyl and pyrimidinyl groups are oriented essentially orthogonally, with a C11—S1—C10—C9 torsion angle of 85.1 (1)°. The aryl rings are inclined to each other at a dihedral angle of 70.5 (3)°. The bond dimensions (Table 1) are within the range reported in analogous compounds (Zhang *et al.*, 2005).

Neither intermolecular hydrogen-bonding nor π–π interactions are found in the crystal packing, though there are two aromatic heterocyclic groups in the molecule of (I).

Experimental

8-Bromomethylquinoline was prepared according to the reported procedure (Dalley *et al.*, 2001). 2-Mercaptopyrimidine (1.0 g, 8.9 mmol) and KOH (0.5 g, 8.9 mmol) were refluxed in ethanol (30 ml) for 1 h; 8-bromomethylquinoline (2.0 g, 9.0 mmol) in THF (15 ml) was then added dropwise. A white precipitate appeared. After stirring under reflux for 5 h, the mixture was cooled to room temperature and the precipitate was filtered off. The filtrate was evaporated to dryness under vacuum and the residue was taken up in the minimum amount of 1:2 dichloromethane/acetone in volume, filtered and allowed to stand. Yellow single crystals of (I) suitable for

X-ray diffraction were obtained by slow evaporation of this solution at room temperature.

Crystal data

$C_{14}H_{11}N_3S$
$M_r = 253.33$
Monoclinic, $P2_1/c$
$a = 9.5743$ (19) Å
$b = 8.0531$ (16) Å
$c = 15.951$ (3) Å
$\beta = 96.60$ (3)°
$V = 1221.8$ (4) Å^3
$Z = 4$
$D_x = 1.377$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.25$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.33 × 0.14 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.915$, $T_{max} = 0.980$
9759 measured reflections
2269 independent reflections
1889 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.095$
$S = 1.02$
2269 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.1251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C10	1.8159 (16)	C9—C10	1.497 (2)
S1—C11	1.7568 (16)		
C11—S1—C10	103.20 (7)		

H atoms were positioned geometrically with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2004).

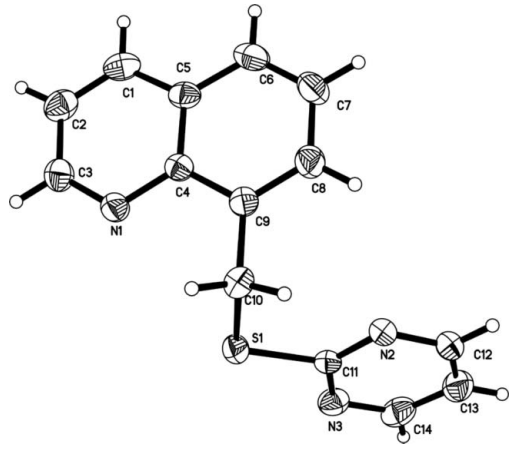


Figure 1
ORTEPII (Johnson, 1976) view of (I), showing atom displacement ellipsoids at the 30% probability level.

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